ECE 659 EXAM V
Tuesday May 6, 2014, FRNY B124 8-10AM

NAME: ____________________________

CLOSED BOOK
All five questions carry equal weight

Please show all work.
No credit for just writing down the answer, even if correct.
5.1.

Consider a channel exchanging electrons and energies with three reservoirs as shown.

(a) What relationship among the different quantities ($N_1$, $N_2$, $E_1$, $E_2$, $E_0$) is required by
(i) Conservation of number of electrons
(ii) Conservation of energy
(iii) Second law of thermodynamics:

(b) Is our current formula for an elastic resistor

$$I = \frac{1}{q} \int dE \, G(E) \left( f_1(E) - f_2(E) \right)$$

in compliance with the second law? Explain

**SOLUTION:**

Please see introductory material (before Section 16.1) in Lecture 16 of Text (LNE)
5.2. Consider a system having three degenerate levels with energy $\epsilon$ having an electron-electron interaction energy related to the number of electrons $N$ by the relation

$$ U(N) = \frac{U_0}{2} N(N-1) $$

At what values of the electrochemical potential $\mu$, will the equilibrium number of electrons change from 0 to 1, from 1 to 2 and from 2 to 3?

**SOLUTION:**

<table>
<thead>
<tr>
<th>States</th>
<th>$E_i - \mu N_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>000</td>
<td>0</td>
</tr>
<tr>
<td>001,010,100</td>
<td>$\epsilon - \mu$</td>
</tr>
<tr>
<td>011,101,110</td>
<td>$2\epsilon + U_0 - 2\mu$</td>
</tr>
<tr>
<td>111</td>
<td>$3\epsilon + 3U_0 - 3\mu$</td>
</tr>
</tbody>
</table>

Transition from $N=0$ to $N=1$ occurs when

$$ \epsilon - \mu_1 = 0 \rightarrow \mu_1 = \epsilon $$

Transition from $N=1$ to $N=2$ occurs when

$$ \epsilon - \mu_2 = 2\epsilon + U_0 - 2\mu_2 \rightarrow \mu_2 = \epsilon + U_0 $$

Transition from $N=2$ to $N=3$ occurs when

$$ 3\epsilon + 3U_0 - 3\mu_3 = 2\epsilon + U_0 - 2\mu_3 \rightarrow \mu_3 = \epsilon + 2U_0 $$
5.3. Consider a single quantum dot with just one level with energy $\varepsilon$. We wish to find the current as a function of the electrochemical potential $\mu_2 = \mu_1 + qV$ (keeping $\mu_1$ fixed) using the Fock space picture by writing

$$\frac{d}{dt} \begin{bmatrix} P_0 \\ P_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} W_1 + W_2 \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \end{bmatrix}$$

where the $W_1$ and $W_2$ matrices describe the transition rates between the different states due to electron exchange with contacts 1 and 2 respectively which are held in equilibrium with electrochemical potentials $\mu_1$ and $\mu_2$.

(a) Write down the matrices $W_1$ and $W_2$ in terms of the Fermi functions in contacts 1, 2.
(b) Obtain the steady-state probabilities $P_0$ and $P_1$.
(c) Obtain the steady-state current.

**SOLUTION:**

(a) 

$$W_1 = \gamma_1 \begin{bmatrix} -f_1 & 1-f_1 \\ +f_1 & -(1-f_1) \end{bmatrix} \quad W_2 = \gamma_2 \begin{bmatrix} -f_2 & 1-f_2 \\ +f_2 & -(1-f_2) \end{bmatrix}$$

(b) 

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} -\gamma_1 f_1 - \gamma_2 f_2 & \gamma_1 (1-f_1) + \gamma_2 (1-f_2) \\ \gamma_1 f_1 + \gamma_2 f_2 & -\gamma_1 (1-f_1) - \gamma_2 (1-f_2) \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \end{bmatrix}$$

$$\frac{P_1}{P_0} = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1(1-f_1) + \gamma_2(1-f_2)} \quad \Rightarrow \quad P_1 = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}, \quad P_0 = 1 - P_1$$

(c) 

$$I = q\gamma_1 \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} -f_1 & 1-f_1 \\ +f_1 & -(1-f_1) \end{bmatrix} \begin{bmatrix} P_0 \\ P_1 \end{bmatrix} = q\gamma_1 (f_1 P_0 - (1-f_1)P_1) = \gamma_1 (f_1 - P_1)$$

$$= q\gamma_1 \left( f_1 - \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right) = q\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$
5.4. Consider two coupled quantum dots each with two spin-degenerate levels, described by the one-electron Hamiltonian,

\[
h = \begin{bmatrix}
\mu & u_1 & u_2 & d_1 & d_2 \\
\epsilon & t & 0 & 0 & 0 \\
t & \epsilon & 0 & 0 & 0 \\
0 & 0 & \epsilon & t & 0 \\
0 & 0 & t & \epsilon & 0 \\
\end{bmatrix}
\]

having an intra-dot interaction energy \(U\) and zero inter-dot interaction energy. Write down the matrices whose eigenvalues will give you the energies of the

(a) \textbf{Zero-electron} states
(b) \textbf{One-electron} states
(c) \textbf{Two-electron} states
(d) \textbf{Three-electron} states
(a) \textbf{Four-electron} states

\textbf{SOLUTION:}

(a) \textbf{Zero-electron} states
\[H_0 = \begin{bmatrix} 0 \end{bmatrix}\]

(b) \textbf{One-electron} states
\[H_1 = h = \begin{bmatrix}
\mu & u_1 & u_2 & d_1 & d_2 \\
\epsilon & t & 0 & 0 & 0 \\
t & \epsilon & 0 & 0 & 0 \\
0 & 0 & \epsilon & t & 0 \\
0 & 0 & t & \epsilon & 0 \\
\end{bmatrix}\]

(c) \textbf{Two-electron states}
\[H_2 = \begin{bmatrix}
u_{1d_1} & u_{1d_2} & u_{2d_1} & u_{2d_2} & u_{1u_2} & d_{1d_2} \\
2\epsilon + U & 0 & t & t & 0 & 0 \\
0 & 2\epsilon + U & t & t & 0 & 0 \\
t & t & 2\epsilon & 0 & 0 & 0 \\
t & t & 0 & 2\epsilon & 0 & 0 \\
0 & 0 & 0 & 0 & 2\epsilon & 0 \\
0 & 0 & 0 & 0 & 0 & 2\epsilon \\
\end{bmatrix}\]
(d) Three-electron states

\[
H_3 = \begin{bmatrix}
  u_2 d_1 d_2 & u_1 d_1 d_2 & u_1 u_2 d_2 & u_1 u_2 d_1 \\
  3\epsilon + U & t & 0 & 0 \\
  t & 3\epsilon + U & 0 & 0 \\
  0 & 0 & 3\epsilon + U & t \\
  0 & 0 & t & 3\epsilon + U \\
\end{bmatrix}
\]

(e) Four-electron states

\[
u_1 u_2 d_1 d_2 \\
[2\epsilon + 2U]
\]
5.5. What is the entropy per spin (\( \rho \): density matrix)

\[
S = -k \, \text{Trace}[\rho \ln \rho]
\]

corresponding to a collection of spins,

(a) 50% of which point along +x and 50% along -x?

(b) 75% of which point along +x and 25% along -x?

(c) 100% of which point along +x?

Note: Wavefunction for (a) spin along +x: \( \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \), (b) for spin along -x: \( \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \)

SOLUTION:

(a) \( \rho = 0.5 \times \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + 0.5 \times \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \)

\[
S = -k \, \text{Trace} \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} \ln 1/2 & 0 \\ 0 & \ln 1/2 \end{pmatrix} = k \ln 2
\]

(b) \( \rho = 0.75 \times \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + 0.25 \times \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1/2 & 1/4 \\ 1/4 & 1/2 \end{pmatrix} \)

Diagonalizing

\[
\rho = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}
\]

Hence

\[
S = -k \, \text{Trace} \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix} \begin{pmatrix} \ln 3/4 & 0 \\ 0 & \ln 1/4 \end{pmatrix} = -k \left( \frac{3}{4} \ln 3/4 + \frac{1}{4} \ln 1/4 \right)
\]

(c) \( \rho = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \)

Diagonalizing

\[
\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}
\]

Hence

\[
S = -k \, \text{Trace} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \ln 1 & 0 \\ 0 & \ln 0 \end{pmatrix} = 0
\]